

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 13, 2013, No. 2



THREE-DIMENSIONAL ADAPTIVE ALGORITHM FOR CONTINUOUS APPROXIMATIONS OF MATERIAL DATA USING SPACE PROJECTION

PIOTR GURGUL*, MARCIN SIENIEK, MACIEJ PASZYŃSKI, ŁUKASZ MADEJ

AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Krakow, Poland *Corresponding author: pgurgul@agh.edu.pl

Abstract

The concept of the H1 projections for an adaptive generation of a continuous approximation of an input 3D image in the finite element (FE) framework is describe and utilized in this paper. Such an approximation, along with a corresponding FE mesh, can be interpreted and used as an input data for FE solvers. In order to capture FE solution gradients properly, specific refined meshes have to be created. The projection operator is applied iteratively on a series of increasingly refined meshes, resulting in an improving fidelity of the approximation. A developed algorithm for linking image processing to the 3D FEM code is also presented within the paper. In particular we compare hp-adaptive algorithm with h-adaptivity, concluding that hp-adaptivity for three dimensional approximation of non-continuous data loses its exponential convergence. Finally conclusions with the evaluation and discussion of the numerical results for an exemplary problem and convergence rates obtained for described problem are described.

Key words: adaptive finite element method, space projections, digital material representation

1. INTRODUCTION

Space projections constitute an important tool, which can be used in diverse applications including finite element (FE) analysis (Demkowicz, 2004; Demkowicz & Buffa, 2004; Demkowicz et. al., 2006). It might be used, for example, to create an approximation of a generic bitmap in the finite element space. Such bitmaps can represent e.g. morphology of the digital material representation (DMR) during FE analysis of material behavior under deformation and exploitation conditions (Madej et al., 2011; Madej, 2010; Paszyński et al., 2005). Due to the crystallographic nature of polycrystalline material, particular features are characterized by different properties that significantly influence material deformation. To properly capture FE solution gradients which are the results of mentioned material inhomogeneities, specific refined meshes have to be created.

The operator can be applied iteratively on a series of increasingly refined meshes, resulting in an improving fidelity of the approximation. A proof of concept for a limited set of applications has been presented in earlier author's works: (Gurgul et al., 2011; Sieniek et al., 2010; Gurgul et al., 2012).

The continuous data approximation, namely the H1 projection, is necessary in case of a noncontinuous input data representing continuous phenomena. Some examples may involve:

- satellite images of topography of the terrain, when we have a non-continuous bitmap data representing rather continuous terrain;
- input data obtained by using various techniques representing temperature distribution over the

material, where the temperature is rather continuous phenomena.

The exemplary application of the first case may involve the flood modeling (Collier et al., 2011), the application of the second case concerns the solution of time dependent problems with input data representing initial conditions. When we solve the nonstationary problems of the form $\frac{\partial u}{\partial t} - \nabla K \nabla u = f$, where u represents temperature, with initial conditions u(x,0)=u₀, where u₀ is represented by a noncontinuous input data, it is rather necessary to perform H¹ projection of the u₀ to get the required regularity of u.

A number of adaptive algorithms for finite element mesh refinements are known. HP-adaptation is one of the most complex and accurate, as it results in an exponential convergence with the number of degrees of freedom (Demkowicz et al., 2006). The hpadaptation process breaks selected finite elements into smaller ones and modifies the polynomial order of approximation locally. H-adaptive algorithm restricts the mesh refinement process to breaking selected finite elements with the fixed polynomial order of approximation, and it results in algebraic convergence only. In this work we compare hpadaptivity with h-adaptivity for the H¹ projection of non-continuous data. We conclude that for three dimensional H¹ projection of continuous data the hpadaptivity loses its exponential convergence and thus h-adaptation is enough.

2. PROJECTION OPERATOR

A L^2 projection onto the space V may be expressed as the following minimization problem: Given an arbitrary function f(x), find $u^{V(x)} \in V$ such that $\| f(x) - u^{V(x)} \|_{L^2(\Omega)}$ is minimal.

Since $u^{V(x)} = \sum_{i=1}^{n} N_i(x) U_i$ where $\{N_i(x)\}_{i=1..n}$ are basis functions for V (i.e. $(span(\{N_i\}_{i=1...n}) = V)$, we have to determine $\{U_i\}_{i=1..n}$, the coefficients of this linear combination.

Given $\|f(x)\|_{L^2} = \int_{\Omega} f(x)d\Omega$, to find the minimum, we differentiate the equation with respect to the coefficients and compare them to zero in equation (1):

$$\frac{\partial}{\partial U_i} \left[\int_{\Omega} \left(f(x) - \sum_{i=1}^n N_i(x) U_i \right)^2 d\Omega \right] = 0 \quad (1)$$

This leads to a linear system (2):

$$M U = F \tag{2}$$

where:

$$M_{j,i} = \int_{\Omega} N_j(x) N_i(x) d\,\Omega \tag{3}$$

$$F_j = \int_{\Omega} f(x) N_j(x) d\,\Omega \tag{4}$$

An L^2 projection onto the space V, $u^{V(x)}$ constitutes the solution to this system.

However, the method above considers only the function itself for minimization of the error. We can include information about derivatives and though minimize not only the error of function's value, but also its gradients. This method is called H^1 projection and can be expressed very similarly to L^2 projection.

Given an arbitrary function f(x), find $u^{V(x)} \in V$ such that

$$\min \| f(x) - u^{V(x)} \|_{H^1(\Omega)}.$$
 (5)

Thus the equation (6)

$$\int_{\Omega} (\mathbf{f}(\mathbf{x}) - \mathbf{u}^{\mathbf{V}(\mathbf{x})})^2 d\,\Omega + \,\alpha \int_{\Omega} (\nabla \mathbf{f}(\mathbf{x}) - \nabla \mathbf{u}^{\mathbf{V}(\mathbf{x})})^2 d\,\Omega.$$
 (6)

needs to be minimal.

Since the material data is not continuous in our case, we need to approximate the partial derivatives in the gradient ∇f by finite differences. For a given X = (x_1, x_2, x_3) , we find the closest existing (integer) coordinates for x_1, x_2, x_3 that are produced by the function r(x). Then, we compute the approximation of $\nabla f(x)$, compare equation (7).

$$\nabla f(\mathbf{x}) \approx \left(\frac{f(\mathbf{r}(\mathbf{x}_1 + \mathbf{h})) - f(\mathbf{r}(\mathbf{x}_1))}{h}; \frac{f(\mathbf{r}(\mathbf{x}_2 + \mathbf{h})) - f(\mathbf{r}(\mathbf{x}_2))}{h}; \frac{f(\mathbf{r}(\mathbf{x}_3 + \mathbf{h})) - f(\mathbf{r}(\mathbf{x}_3))}{h}\right)$$
(7)

3. ADAPTIVE ALGORITHM USED FOR SOLUTION

Quality of the approximation depends on the choice of the space V, where the approximation will be performed. There is no efficient way to determine precision of a given V a priori and a workaround here is to refine space V iteratively, based on relative error rate in each step. This is done using self-containing spaces $\{V_t\}_{t=1,...,m}$ where V_1 corresponds to the initial mesh and V_m is the first mesh, for which the desired precision is achieved. Let:

 u^V be a solution in the space V,

_

1: $u^{V_t} \leftarrow$ solve the minimization problem in V_t

2:
$$V_t^{fine} \leftarrow V_t$$

3: $u^{V_t^{fine}} \leftarrow$ solve the minimization problem in

$$V_t^{fine}$$

4: $max_err \leftarrow 0$

5: foreach element *K* in coarse mesh do

6:
$$V_t^{opt} \leftarrow V_t^{fine}$$

7: foreach $V_t \subset V_t^w \subseteq V_t^{fine}$ over element *K*

such that $|V_t^w|_K - |V|_K \neq 0$ do

8: $u^{V_t^{opt}} \leftarrow \text{compute a projection of } u^{V_t^{fine}} \text{ onto}$ V_t^{fine}

```
9:
```

$$err(V_{t}^{w},K) \leftarrow \frac{\left\| u^{v_{t}^{fine}} - u^{v_{t}} \right\|_{H^{1}(K)} - \left\| u^{v_{t}^{fine}} - u^{v_{t}^{w}} \right\|_{H^{1}(K)}}{|v_{t}^{w}|_{K} - |v|_{K}}$$

- 10: if $err(V_t^w, K) < err(V_t^{opt}, K)$ then
- 11: $V_t^{opt} \leftarrow V_t^w$
- 12: end if
- 13: end for
- 14: add all basis functions from V_t^{opt} with supports

on K to V_{t+1}

- 15: **if** $err(V_t^w, K) > max_err$
- 16: $\max_err \leftarrow err(V_t^w, K)$
- 17: **end if**
- 18: end for
- 19: return V_{t+1} , max_err

Fig. 1. Choice of an optimal mesh for the following iteration of the adaptive algorithm.

- V_t^{fine} be a space corresponding to a mesh, where all elements have been refined by one order with respect to V_t ,
- V_t^{opt} be a space corresponding to a mesh, where element refinements have been optimally chosen by comparing V_t^{fine} and V_t ,
- V_t^w be any space such that $V_t \subset V_t^w \subseteq V_t^{fine}$.
- Major steps of described algorithm are presented in figure 1.

Algorithm presented in figure 1 is being performed in iterations until the stop condition (usually the desired precision) is met. These steps are presented in figure 2.

1:
$$err \leftarrow \infty$$

2:
$$t \leftarrow 1$$

- 3: $V_t \leftarrow$ initial space corresponding to a trivial mesh
- 4: while err > desired_precision do
- 5: V_{t+1} , err \leftarrow perform listing 1 on V_t
- 6: $V_t \leftarrow V_{t+1}$
- 7: $t \leftarrow t + 1$
- 8: end while
- 9: return V_{t+1}

Fig. 2. Algorithm approximating space V with the desired_precision.

3.1. HP Mesh refinements and its role in projection-based interpolation

The quality of the interpolation can be improved by the expansion of the interpolation base. In FEM terms, this could be done thanks to some kind of mesh adaptation. Two methods of adaptation are being considered in the present work:

3.1.2. *P-adaptation* – increasing polynomial approximation level. One approach is to increase order of the basis functions on the elements where the error rate is higher than desired. More functions in the base means smoother and more accurate solution but also more computations and the use of high-order polynomials.

3.1.3. H-adaptation – refining the mesh. Another way is to split the element into smaller ones in order to obtain finer mesh. This idea arose from the observation that the domain is usually non-uniform and in order to approximate the solution fairly some places require more precise computations than others, where the acceptable solution can be achieved using small number of elements. The crucial factor in achieving optimal results is to decide if a given element should be split into two parts horizontally, into two parts vertically, into four parts (both horizontally and vertically on one side), into eight parts (both horizontally and vertically on the both sides) or not split at all. That is why the automated algorithm that decides after each iteration for the element if it needs h- or p-refinement or not was developed. The refinement process is fairly simple in 1D but the 2D and 3D cases enforce a few refinement rules to follow.

3.1.4. Automated hp-adaptation algorithm

Neither the p- nor the h-adaptation guarantees error rate decreases in an exponential manner with a step number. This can be achieved by combining together mentioned two methods under some conditions, which are not necessarily satisfied in the present case. Still, in order to locate the most sensitive areas at each stage dynamically, and improve the solution as much as possible, the self-adaptive algorithm can be applied. It decides if a given element should be refined or it is already properly refined for the satisfactory interpolation, in an analogical manner to the algorithm for Finite Elements adaptivity described by (Demkowicz et al., 2006).

4. NUMERICAL RESULTS

Presented projection algorithm was tested on one three dimensional example, with hp-adaptive (see figure 3) and h-adaptive (see figure 4) algorithms. The example concerns the approximation of the input data representing the ball shape distribution of data. This may represent the initial distribution of temperature over one ball shape material inside another material. This temperature distribution may constitute the starting point for some non-stationary time dependent heat transfer simulation.

The numerical results presented in table 1 obtained by the hp-adaptive solution show that the algorithm utilized for the three dimensional H1 projections does not deliver exponential convergence, and thus it is reasonable to replace it with its cheaper, h-adaptivite counterpart that delivers similar convergence to the one presented in table 2, with simpler implementation and longer execution time.

Table 1. Convergence rate for the problem of H^l projections of 3D balls with hp-adaptivity.

| Iteration | Mesh size | Relative error in H ¹ norm |
|-----------|-----------|---------------------------------------|
| 1 | 125 | 71.3 |
| 2 | 2197 | 66.3 |
| 3 | 5197 | 62.4 |
| 4 | 12093 | 63.9 |
| 5 | 22145 | 57.7 |
| 6 | 41411 | 51.03 |



Fig. 3. 3D balls problem: mesh after the sixth iterations of hp adaptive algorithm and solution over the mesh.



Fig. 4. 3D balls problem: mesh after the sixth iterations of the h-adaptive algorithm and solution over the mesh.

Table 2. Convergence rate for the problem of H^1 projections for 3D balls with h-adaptivity.

| Iteration | Mesh size | Relative error in H ¹ norm |
|-----------|-----------|---------------------------------------|
| 1 | 125 | 72.1 |
| 2 | 729 | 68.3 |
| 3 | 4913 | 68.2 |
| 4 | 11745 | 62.1 |
| 5 | 32305 | 52.9 |
| 6 | 68257 | 49.44 |

5. CONCLUSIONS AND FUTURE WORK

This paper presents a way of incorporating wellestablished H^1 projection concept into an adaptive algorithm used to prepare material data. The described method allows for generation of a smooth, continuous interpolation of given arbitrary data, alongside with an initial pre-adapted mesh suitable for further processing by a non-stationary FE solver.

In this paper we compared three dimensional hpadaptivity with h-adaptivity, concluding that the hpadaptive algorithm does not deliver the exponential convergence in the case of non-continuous approximation of data, and it may be reasonable to utilize just h-adaptation algorithm, with uniform polynomial order of approximation, which is significantly easier to implement.

It is desirable to experiment with more 3D images as well as with various input parameters (e.g. boundary conditions or image conversion algorithms). Besides, more sophisticated digital material representations should be investigated. The applicability of this methodology for non-stationary finite element method solvers will be tested in our future work. In particular we plan to test the influence of the quality of projection of the initial state to the further stability of the non-stationary simulation.

Acknowledgements. The work of the first author was partly supported by The European Union by means of European Social Fund, PO KL Priority IV: Higher Education and Research, Activity 4.1: Improvement and Development of Didactic Potential of the University and Increasing Number of Students of the Faculties Crucial for the National Economy Based on Knowledge, Subactivity 4.1.1: Improvement of the Didactic Potential of the AGH University of Science and Technology "Human Assets", No. UDA - POKL.04.01.01-00-367/08-00. The work of the second author was supported by Polish National Science Center grants no. DEC-2011/03/N/ST6/ 01397. The work of the third author was supported by Polish National Science Center grant no. NN519447739. The work of the fourth author was supported by grant no. nr 820/N-Czechy 2010/0.

REFERENCES

- Collier, N., Radwan, H., Dalcin, L., 2011, Time Adaptivity in the Diffusive Wave Approximation to the Shallow Water Equations, *accepted to Journal of Computational Science*.
- Demkowicz, L., Kurtz, J., Pardo, D., Paszyński, M., Zdunek, A., 2006, *Computing With Hp-adaptive Finite Elements*, CRC Press, Taylor and Francis.
- Demkowicz, L., Buffa, A., 2004, H¹, H(curl) and H(div) conforming projection-based interpolation in three dimensions, *ICES-Report 04-24*, The University of Texas in Austin.
- Demkowicz, L., 2004, Projection-based interpolation, ICES Report 04-03, The University of Texas in Austin.
- Gurgul, P., Sieniek, M., Magiera, K., Skotniczny, M., 2011, Application of multi-agent paradigm to hp-adaptive projection-based interpolation operator, *accepted to Journal of Computational Science*.
- Gurgul, P., Sieniek, M., Paszyński, M., Madej, Ł., Collier, N., 2012, Two dimensional hp-adaptive algorithm for con-

tinuous approximations of material data using space projections; accepted to Computer Science.

- Madej, L., 2010, Development of the modeling strategy for the strain localization simulation based on the Digital Material Representation, DSc dissertation, AGH University Press, Krakow.
- Madej, L., Rauch, L., Perzyński, K., Cybułka P., 2011, Digital Material Representation as
- an efficient tool for strain inhomogeneities analysis at the micro scale level, *Archives of Civil and Mechanical Engineering*, 11, 661-679.
- Paszyński, M., Romkes, A., Collister, E., Meiring, J., Demkowicz, L., Wilson, C.G., 2005, One the modeling of Step-and-Flash imprint lithography using molecular static models, *ICES-Report 05-38*.
- Perzyński, K., Major, Ł., Madej, Ł., Pietrzyk, M., 2011, Analysis of the stress concentration in the nanomultilayer coatings based on digital Representation of the structure, *Archives of Metallurgy and Materials*, 56, 393-399.
- Sieniek, M., Gurgul, P., Kołodziejczyk, P., Paszyński, M., 2010, Agent-based parallel system for numerical computations, *Procedia Computer Science*, 1, 1971-1981.

TRÓJWYMIAROWY, ADAPTACYJNY ALGORYTM DO APROKSYMACJI CIĄGŁYCH DANYCH MATERIAŁOWYCH Z WYKORZYSTANIEM PROJEKCJI PRZESTRZENNYCH

Streszczenie

Celem niniejszego artykułu jest opis i pokazanie praktycznego wykorzystana koncepcji projekcji H¹ do adaptacyjnej generacji aproksymacji ciągłej wejściowego obrazu w 3D w bazie elementów skończonych. Taka aproksymacja, razem z odpowiadającą jej siatką, może być interpretowana jako ciągła reprezentacja danych wejściowych dla solwerów metody elementów skończonych (MES).

Artykuł przedstawia teoretyczne podstawy mechanizmu projekcji wraz z porównaniem algorytmów hp- adaptacji i h-adaptacji użytych do iteracyjnego generowania kolejnych aproksymacji. Omówiony został również sposób oszacowania i redukcji błędu aproksymacji. Przedstawiony został ponadto przykład obliczeniowy ilustrujący działanie opisywanych metod.

> Received: September 26, 2012 Received in a revised form: October 23, 2012 Accepted: October 26, 2012

